GENÍS LLEOPART MOTIS

Physicist Researcher & Ph.D. in Computational Chemistry

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EXPERIENCE

Researcher

Istituto Officina dei Materiali (IOM-CNR)

June 2024 – Ongoing Cagliari, Italy

- Theoretical and computational modelling study of highly relevant nanomaterials such as perovskites, double-perovskites, and 2D semiconductors with potential applications in the industry.
- Collaboration with experimentalists, merging experimental data with theoretically predicted results for deep scientific comprehension of materials' phenomena.
- Development of **Machine Learning** force-fields on double-perovskites and other systems for classical MD simulations and magnetic predictions.

Pre-doctoral researcher in Computational Chemistry

Universitat de Barcelona

June 2019 – 2024 Barcelona

- Defended Ph.D. thesis entitled "Computational modelling of 2D carbon-based materials with tunable electronic properties", supervised by Prof. Dr. Stefan T. Bromley and Prof. Dr. Ibério de P. R. Moreira. Grade: Cum Laude.
- **Presented my research** at national and international conferences (poster and 20 – 60 min oral presentations in English). Won the Prize for the best poster and research project at the Scientific Advisory Board Meeting in 2019.
- **Did outreach** to non-scientific community.
- **Created collaborations** with other international research groups, such as Prof. Dr. Roser Valentí's group in Frankfurt.
- Development of two patents on 2D carbon-based materials in colaboration with IDEADED.
- HPC-Europe fellowship in 2021 for stay abroad with project entitled "Establishing an efficient framework for modelling correlated states in 2D graphenic systems by combining DFT and Many-Body Methods".

Teaching assistant

Universitat de Barcelona

Oct 2020 – Feb 2024 Barcelona

- Programming courses to 1st year Chemistry undergrad students. The courses comprised Python and introduction to Computational Modelling of chemistry toy models.
- Taught, assisted, prepared exercises and evaluated students (∼ 15 students/course)

EDUCATION

Master (M.Sc.) in Atomistic computational modeling of physical, chemical and biochemical systems.

Universitat de Barcelona (UB)/Universitat Politècnica de Catalunya (UPC)

Sept 2017 – Sept 2018 Barcelona

- UBICS Scholarship and worked as a researcher during the final master thesis, "Simulated quantum annealing of a frustrated Hamiltonian in random networks", supervised by Dr. Matteo Palassini.

Bachelor degree (B.Sc.) in Physics

Universitat de Barcelona

Sept 2012 – July 2016 Barcelona

LANGUAGES

	A2	B1	B2	C1	C2
Catalan	●	●	●	●	●
Spanish	●	●	●	●	●
English	●	●	●	●	○
Italian	●	●	●	●	○
French	●	○	○	○	○
German	●	○	○	○	○

SOFTWARE

MS Office
Excel, Word, PowerPoint

Programming
Matlab, Fortran, Python, C++, Javascript, Julia, Bash, Perl

Computational Modelling
FHI-Aims, ASE, VASP, Quantum Espresso, Wannier90, CRYSTAL09/17, SIESTA, ABINIT, GAUSSIAN

Others
LaTeX, Adobe Illustrator, Gnuplot

TECHNICAL SKILLS

Complex problem-solving · Critical thinking · Communication · Project management · Collaboration & temwork · Adaptability & learning · Leadership & mentoring · Data Visualization · Machine Learning · Pattern Recognition · Database Structures & Algorithms · Data Preparation